

Quasiparticles and c-axis coherent hopping in high T_c superconductors

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We study the problem of the low-energy quasiparticle spectrum of the extended t - J model and analyze the coherent hopping between weakly coupled planes described by this model. Starting with a two-band model describing the CuO planes and the unoccupied bands associated to the metallic atoms located in between the planes, we obtain effective hopping matrix elements describing the c -axis charge transfer. A computational study of these processes shows an anomalously large charge anisotropy for doping concentrations around and below the optimal doping.

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The anomalous charge transport of high T_c materials is still among the most important open problems related with the physics of these compounds [1,2]. It is now accepted that in order to build a complete theory of high temperature superconductivity, a deep understanding of the normal state properties of these compounds is needed and one of the most intriguing questions concerns precisely the charge dynamics [3]. The cuprate high T_c superconductors have crystalline structures consisting of CuO planes which makes all of them highly anisotropic materials. The electrical conductivity reflects the anisotropy: while in the plane it shows a metallic behavior, along the c -axis in the underdoped regime, it indicates an incoherent charge transport; moreover, it has an anomalous temperature behavior, and its frequency dependence is not of the Drude type [4].

Band structure calculations together with a semiclassical theory of charge transport, predict a metallic behavior in all directions with an anisotropy much smaller than the experimental values. Electron-electron interactions may strongly renormalize the bare parameters, however within the framework of the Fermi-liquid theory the observed anisotropy cannot be understood. This led Anderson and others to propose the failure of the conventional Fermi-liquid theory in these compounds [5].

An important amount of experimental data has been accumulated during the last years [6]. Among other things, the formation of charge stripes in the normal state has been confirmed [7]. Whether this is relevant for the occurrence of superconductivity is not yet clear, however it should be taken into account in a detailed description of the normal phase.

Here we revisit the problem of the low-energy quasiparticle spectrum of the extended t - J model and analyze the coherent hopping between weakly coupled planes. Our starting point is a stack of CuO planes coupled via the electron hopping $t_\perp(\mathbf{k})$ to higher energy intermediate states. The intermediate states represent the unoccupied bands associated to the metallic atoms located in between the planes.

In a single-particle theory, the intermediate states can

be easily eliminated through a canonical transformation giving rise to an effective hopping between consecutive CuO planes of the form $t_\perp^0(\mathbf{k}) = t_\perp^2(\mathbf{k})/\Delta E_{\mathbf{k}}$, with $\Delta E_{\mathbf{k}}$ the one-particle energy difference between \mathbf{k} -states of the CuO and the intermediate layer bands. The principal symmetry of $t_\perp^0(\mathbf{k})$ is obtained from electronic structure calculations and for the case of $YBaCuO$ it is given by $[\cos(k_x a) - \cos(k_y a)]^2$ [8].

In what follows we use an uncorrelated empty band to describe the intermediate states and the extended t - J model to describe the CuO planes. The extended t - J model including hole hopping to second and third nearest-neighbor (NN) sites, and with J/t consistent with experimental values, reproduces the photoemission results of the parent insulating materials [9,10]. In the standard notation the model Hamiltonian describing the plane l is:

$$H_l = J \sum_{\langle i,j \rangle} \mathbf{S}_{li} \cdot \mathbf{S}_{lj} - \sum_{n,m} t_{nm} c_{ln\sigma}^\dagger c_{lm\sigma} \quad (1)$$

where the matrix element t_{nm} is t for NN, t' for second NN and t'' for third NN, $c_{lm\sigma}$ destroys an electron with spin σ at site m and double occupation is not allowed. Using the many-body states, we perform a canonical transformation that eliminates the intermediate states and generates an effective Hamiltonian that includes a charge transfer matrix element between two consecutive CuO planes. Let us first consider the case of a single hole. The two-plane states of the system are indicated as $|\psi_{0,\nu}^1\rangle \otimes |\psi_{1,\nu'}^2\rangle$ where $|\psi_{m,\nu}^l\rangle$ is the many-body wave function of plane l with m holes and quantum numbers ν and the corresponding energy is $E_{m,\nu}$. We take the plane with no holes in its ground state indicated by $\nu = 0$. The effective matrix elements connecting the states $|\psi_{0,0}^1\rangle \otimes |\psi_{1,\nu}^2\rangle$ and $|\psi_{1,\nu}^1\rangle \otimes |\psi_{0,0}^2\rangle$ accounts for a hopping - from one plane to the other - of a single hole. The one-hole quantum numbers ν include the crystal momentum \mathbf{k} , spin variables and other quantum numbers μ that uniquely identify the state and in what follows we take $\nu \equiv (\mathbf{k}, \sigma, \mu)$. Due to the momentum and spin conservation of the Hamiltonian, the effective hopping of a

hole with momentum \mathbf{k} and spin σ is given by:

$$\tilde{t}_\perp(\mathbf{k}) = \frac{t_\perp^2(\mathbf{k})M_1(\mathbf{k}, \sigma, \mu)M_2^*(\mathbf{k}, \sigma, \mu)}{E_{0,0} - E_{1,(\mathbf{k}, \sigma, \mu)} - \varepsilon_{\mathbf{k}\sigma}} \quad (2)$$

where $\varepsilon_{\mathbf{k}\sigma}$ is the energy to add an electron at the intermediate band, $M_1(\mathbf{k}, \sigma, \mu) = \langle \psi_{1,(\mathbf{k}, \sigma, \mu)}^1 | c_{1\mathbf{k}\sigma} | \psi_{0,0}^1 \rangle$ and $M_2^*(\mathbf{k}, \sigma, \mu) = \langle \psi_{0,0}^2 | c_{2\mathbf{k}\sigma}^\dagger | \psi_{1,(\mathbf{k}, \sigma, \mu)}^2 \rangle$ are the matrix element for the creation and destruction of a hole in the planes. We calculate many-body energies and matrix elements by exact diagonalization of small clusters with periodic boundary conditions.

Consider the one-hole ground state in a 16-site cluster: this state has momentum $\mathbf{k} = (\pi/2, \pi/2)$ and the product of the matrix elements in Eq.(2) is the weight of the quasiparticle peak Z_k . Since the same factor Z_k renormalizes the in-plane hole mass, for one hole close to the Fermi surface, interactions do not renormalize the anisotropy. The one-hole state with $\mathbf{k} = (\pi/2, \pi/2)$ can be viewed as a spin-1/2 and charge e quasiparticle, where the spins across the hole have ferromagnetic correlations. To distinguish this excitation from others that appear at different regions of the Brillouin zone (BZ), we refer to it as the α -type spin-1/2 quasiparticle. This quasiparticle exists for all the momenta in the BZ and its energy can be obtained simply by following the lowest energy peak of the one-particle spectral density, *i.e.* its dispersion relation, shown in Fig.(1), gives the one-hole photoemission (PES) dispersion of the insulator. It is important to note that this quasiparticle is not the lowest energy state for all momenta \mathbf{k} . For realistic parameters that fit the PES ($J/t = 0.4$, $t'/t = -0.35$ and $t''/t = 0.25$), the lowest energy states in the 4×4 cluster with $\mathbf{k} = (0,0)$ and (π, π) have total spin 3/2 [14]. These high spin states have been obtained in clusters of different sizes (up to 20 sites) and for different parameters. However it is not clear that in the thermodynamic limit they will remain being the lowest energy excitations around the Γ and M points. These states can be interpreted as high spin quasiparticles that occur as a precursor of the Nagaoka state. The magnetization is confined around the hole like in a polarized spin bag. These states are not connected to the ground state of the undoped system when a hole is created; in other words the matrix elements in Eq.(2) are zero and these excitations do not propagate - to lowest order - from one plane to the other. The reason is that when a hole is created on the spin-zero ground state of the insulating system, the resulting states have total spin 1/2, and the spin wave function is orthogonal to the spin-3/2 excitations.

More interesting are the one-hole lowest energy states at $\mathbf{k} = (\pi, 0)$ or $(0, \pi)$. These states have been studied recently in some detail [10,11]. The spin correlations across the hole are antiferromagnetic (AFCAH), like in 1D systems, and it has been speculated that this is an indication of charge and spin separation in the 2D t - J model [12].

Similar to the high spin excitation case, here also, the matrix elements connecting this state with the ground state of the undoped system by creating a hole is zero. Although the total spin of the $\mathbf{k} = (\pi, 0)$ lowest energy excitation is 1/2, the symmetry of its spin wave function is orthogonal to that of $c_{1\mathbf{k}\sigma} | \psi_{0,0}^1 \rangle$. The one-hole spectral density of the insulator does not show any structure at the energy of this state as shown in Fig. (2b). Again, to lowest order, this excitation does not propagate from one plane to the other. This is a property of the $tt't'' - J$ model and it is not observed in the t - J model for similar values of J/t .

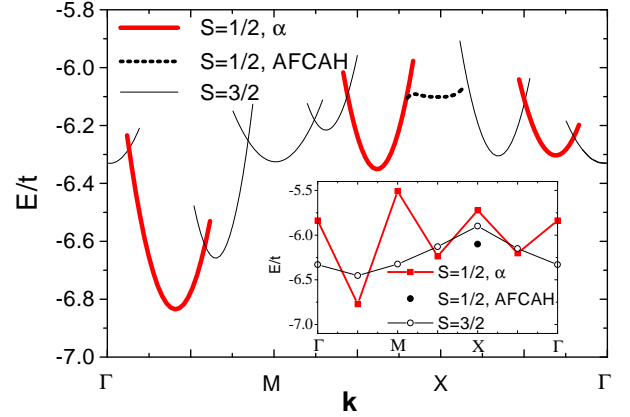


FIG. 1. Dispersion of one hole for the extended t - J model on a 4×4 cluster; $t'/t = -0.35$, $t''/t = 0.25$, and $J/t = 0.4$. In the inset the one hole PES is shown together with the $S = 3/2$ and the AFCAH state energies. Here $\Gamma \equiv (0, 0)$, $M \equiv (\pi, \pi)$, and $X \equiv (\pi, 0)$.

In order to qualitatively determine the regions of the BZ where the different type of excitations are the lowest energy ones, we have continuously changed the boundary conditions in the cluster and the results are shown in Fig. (1). In a region around the X point, the spin-1/2 states with AFCAH are stable (dashed line). If these excitations actually describe a region of charge and spin separation, the dashed line branch does not correspond to the dispersion of a single quasiparticle but to the superposition of a holon and a spinon. It has been suggested that these states play a central role in the many-holes states and may be responsible for the formation of stripes [12]. As we show below, they are also relevant for the coherent hopping along the c -axis in the doped systems.

Summarizing the one-hole results, we have shown that in different regions of the BZ, the lowest energy excitations are of different nature. Close to the Fermi surface ($\mathbf{k} = (\pi/2, \pi/2)$), there is a spin-1/2 quasiparticle that propagates along the c -axis with an effective hopping renormalized with the Z_{k_F} factor. At the X point, the anomalous spin-1/2 excitation with AFCAH is the lowest energy state. A hole in this state is confined, up to second order in t_\perp , in a single plane. Here the word

confinement is used in the sense that there is no bonding-antibonding splitting of the degenerate two-plane lowest energy state. In Fig.(2c) the matrix element for different values of \mathbf{k} is shown. Higher order terms may generate a coherent hopping for this type of excitations. In any case, we expect these higher order terms to generate a very small dispersion along the c -axis [13]. Moreover, it should be noted that for the 20-site cluster, for the $\mathbf{k} = (0, \pi)$ state with robust AFCAH, the second order matrix elements non zero but very small, *i.e.* the quasi-particle peak in the spectral density of the insulator has an extremely small weight [10,11], leading to a strongly renormalized c -axis hopping for this state, in qualitative agreement with the results for the 16-site system. The non-crossing approximation in larger systems also gives zero weight [14].

Let us now turn to the many-holes states. For the same parameters as above, the two-hole ground state of the 4×4 cluster has total momentum $\mathbf{k} = (0, \pi)$ or $(\pi, 0)$ and spin zero. In these states, the hole-hole correlation function $\langle n_i n_j \rangle$ with n_i the hole number at site i , clearly shows the tendency to stripe formation. For the state with $\mathbf{k} = (0, \pi)$ $[(\pi, 0)]$, the holes are mostly aligned in the same row along the x [y] direction as shown in Fig (2d). These results are in agreement with previous results obtained in ladders and clusters. In the 18-site cluster, stripes are observed in the three holes ground state [12]. Based on the spin correlations across the hole, it has been argued that these stripes are made out of one-hole building-blocks with AFCAH [12]. In other words, the two holes wave function has a large component of the one-hole wave function of the $\mathbf{k} = (0, \pi)$ type. This could strongly influence the charge mobility along the c -axis. We first analyze the case of two 4×4 planes with three holes corresponding to a doping $x \simeq 0.094$. With a straightforward extension of the previous treatment and notation, we calculate the effective matrix element mixing the two (degenerate) states with wavefunctions $|\psi_{1,\nu}^1\rangle \otimes |\psi_{2,\xi}^2\rangle$ and $|\psi_{2,\xi}^1\rangle \otimes |\psi_{1,\nu}^2\rangle$ which now are $M_1(\mathbf{k}, \nu, \xi) = \langle \psi_{2,\xi}^1 | c_{1\mathbf{k}\sigma} | \psi_{1,\nu}^1 \rangle$ and $M_2^*(\mathbf{k}, \nu, \xi) = \langle \psi_{1,\nu}^2 | c_{2\mathbf{k}\sigma}^\dagger | \psi_{2,\xi}^2 \rangle$. For these matrix elements to be non zero, the operators $c_{1\mathbf{k}\sigma}$ and $c_{2\mathbf{k}\sigma}^\dagger$ have to be chosen to conserve total momentum and spin.

If the two planes are in their ground state, the product of these matrix elements is smaller than for the one-hole case. This result, is consistent with the conjecture that the two holes wave function is mainly made out of one-hole building blocks with AFCAH since, as we showed above, this type of excitation tends to be confined in one plane. This effect is largely enhanced when doping increases as in the case of five holes in two 4×4 planes ($x \simeq 0.156$). In this case, if the planes are in the ground state, with two and three holes respectively, the effective matrix element to transfer a charge from one plane to the other is exactly zero and to lowest order, charge is

confined in the planes. In fact as shown in Fig. (3b), the PES of the system with two holes has no structure at the energy of the three-hole ground state. The case of four holes ($x = 0.125$) deserves a special comment: the ground state of the uncoupled planes has two holes in each one and the hopping mixes it with excited states. It has been proposed to artificially shift the energy levels of the states with one hole in one plane and three in the other to recover a degeneracy [15]. These shifts are unimportant when calculating the matrix elements which are $\langle \psi_{3,\xi_0}^1 | c_{1\mathbf{k}\sigma} | \psi_{2,\nu_0}^1 \rangle \times \langle \psi_{1,\eta_0}^2 | c_{2\mathbf{k}\sigma}^\dagger | \psi_{2,\nu_0}^2 \rangle$ with the indices ξ_0 , η_0 and ν_0 corresponding to the ground state of a plane with the indicated number of holes. These matrix elements are precisely the ones calculated in the two previous cases and the product is zero. For the case of 6 holes in two 4×4 planes we reach similar conclusions.

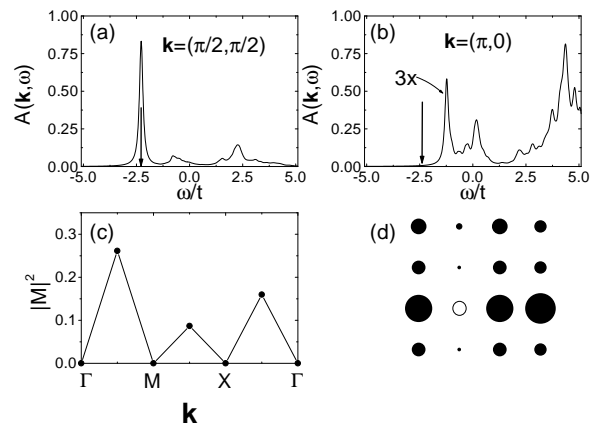


FIG. 2. (a),(b) Single hole spectral functions $A(\mathbf{k}, \omega)$, for the extended t -J model, same parameters as Fig.(1) (broadening $\delta = 0.1t$). The arrow points to the one-hole lowest energy state with the corresponding momentum. (c) Matrix element $|M|^2$ for the available momenta on a 4×4 cluster. (d) Hole density around one hole (open circle) on the two holes ground state ($\mathbf{k} = (0, \pi)$). Full circles radius are proportional to the hole density.

Finally we have evaluated the effective hopping for large number of holes, 9 and 11 holes in the two planes which correspond to dopings x larger than the optimal doping. In this region, the effective hopping calculated always in second order in t_\perp and in the ground state, are non-zero.

We have also studied the effective hopping along the c -axis for 18-site and 20-site clusters, and small doping. For the 18-site cluster, and the same parameters as before, the two holes low energy spectrum presents a quasidegeneracy between the spin zero and spin one states. The effective hopping calculated in the lowest energy $S = 0$ state, which we believe is the relevant in the thermodynamic limit, shows the same behavior as in the 4×4 cluster, indicating that our results are not dominated by the particular symmetry of these clusters.

In Fig. 3(c) we summarize the results for the matrix elements, which give an estimate of ratio $\tilde{t}_\perp/t_\perp^0$ as a function of the doping x , here with t_\perp^0 is the bare hopping obtained from band structure calculations. Our results show that while a single hole propagates along the c -axis, for doping close and smaller than the optimal doping $x_{op} \simeq 0.2$ the lowest order hopping evaluated in the ground state cancels [16] and increases for $x > x_{op}$. This behaviour suggest that when stripes are stabilized, the c -axis hopping reduces to very small values. These results are in agreement with previous calculations [17] which suggest that the weight of the quasiparticle peak decreases in the presence of stripes. As we mentioned above, higher order terms generate a non-zero hopping. However, at least in the one-hole case in the two $\sqrt{8} \times \sqrt{8}$ planes [13], these contributions are very small reducing the bare hopping by a factor smaller than 10^{-3} .

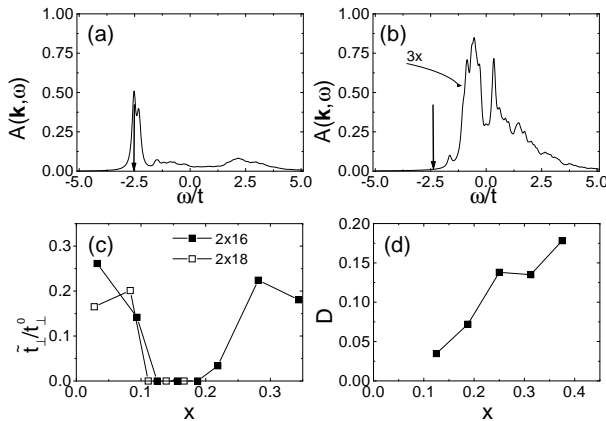


FIG. 3. (a) Single-hole spectral function $A(\mathbf{k}, \omega)$ for a 4×4 cluster with one hole ($\mathbf{k} = (-\pi/2, \pi/2)$), for the extended t-J model and same parameters as Fig (1). The arrow points to the final state energy. (b) Same as (a) for a system with two holes ($\mathbf{k} = (0, 0)$). (c) Effective hopping between CuO planes up to second order in t_\perp as a function of the hole doping x for the 16-site and 18-site clusters. (d) Drude weight averaged over both directions for the 4×4 cluster as a function of the hole doping x .

For the sake of completeness we have also calculated the in-plane Drude weight D for the same parameters as before. As shown in Fig. 3(d) D increases with doping (as in the t-J model [2]) in the region where \tilde{t}_\perp presents a marked depletion. Our treatment, based in a canonical transformation and the estimation of matrix elements by exact diagonalization of small clusters is not appropriate to give a definite answer to what may be the most relevant question related to the charge dynamics in high T_c materials, that is whether under some conditions real confinement of charge excitations in the CuO planes is obtained. However our results are consistent with, and can explain, the available experimental data. The behavior here obtained is robust under changes of the pa-

rameters within the accepted range of values. On one hand, to lowest order in t_\perp , in the ground state charge is confined for doping x close to and below the optimal doping x_{op} . Higher order terms in t_\perp may generate a small coherent hopping $\tilde{t}_\perp \simeq t_\perp \times 10^{-3}$. Estimations of the bare hopping using LDA band structure calculations give $t_\perp = 0.25$ eV for the case of bilayers and $t_\perp \simeq 0.03$ eV for the interplane matrix element [8]. That means that down to very low temperatures ($kT \sim \tilde{t}_\perp$), we expect a diffusive-like propagation along the c -axis with an anomalous temperature dependence. On the other hand, the small cluster calculations are remarkable in the sense that they predict an anomalously large charge anisotropy precisely in the region where superconductivity is stable. This agrees with the experimental data [18] and strengthens the ideas developed by Anderson and coworkers [19] that argued that the lack of single particle intraplane coherent hopping enhances superconductivity.

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